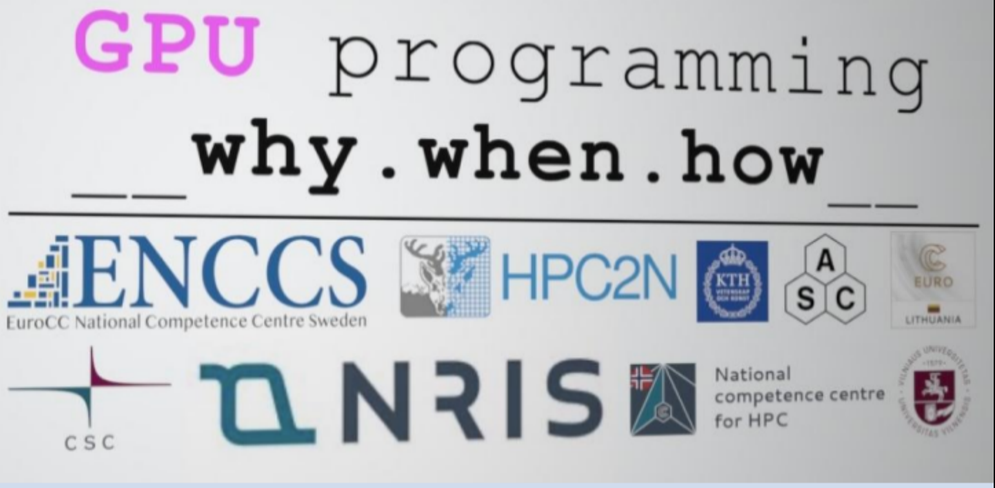
CSC

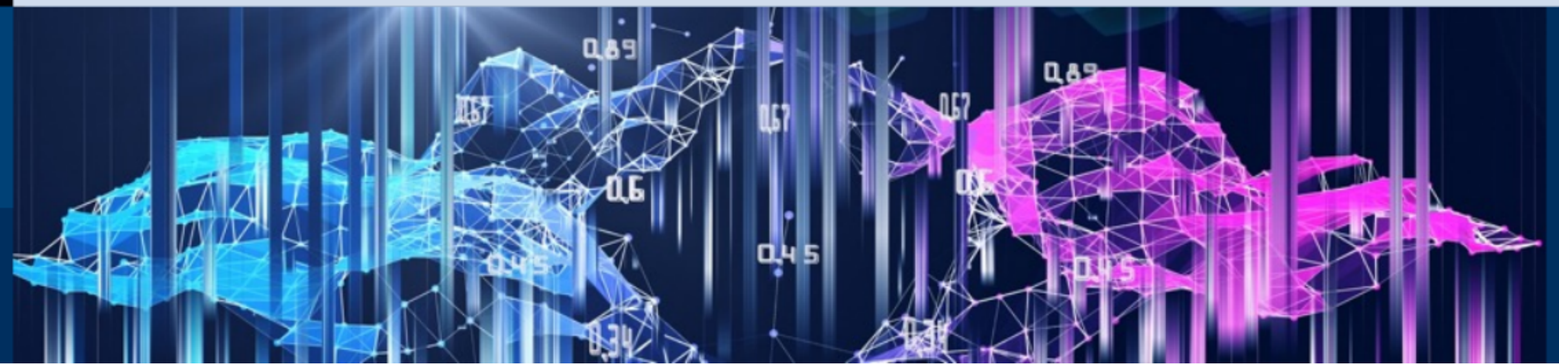
ICT Solutions for Brilliant Minds

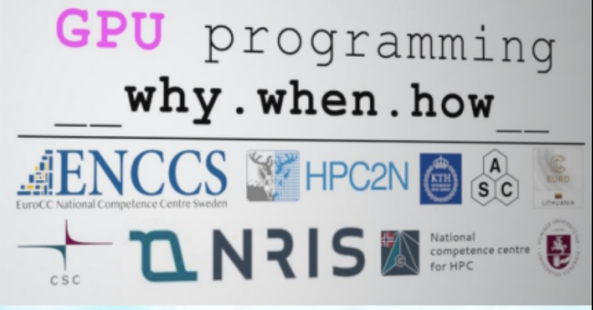


GPU Programming. When, Why and How?

2024

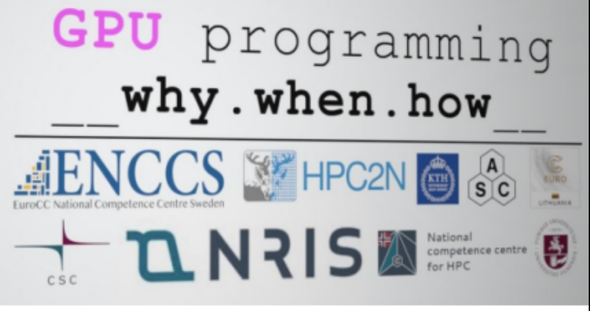
ENCCS Training





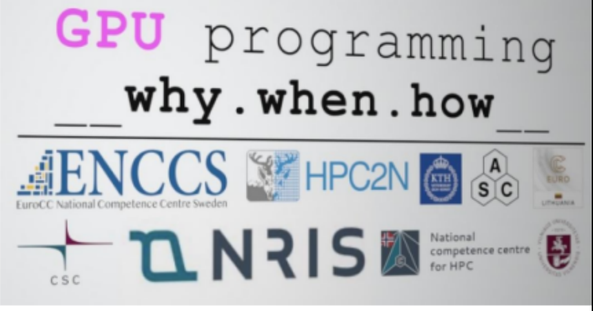
Porting from CPU to GPU

General Considerations



- **Identify Targeted Parts**: The Pareto principle suggests that roughly 10%-20% of the code accounts for 80-90% of the execution time.
- **Equivalent GPU Libraries**: Check for the equivalent GPU libraries that can replace CPU-based libraries.
- **Refactor Loops**: Sometimes loops refactoring is necessary to suit the GPU architecture. Often splitting the loops is necessary.
- **Memory Access Optimization**: GPUs perform best when memory access is coalesced and aligned. Minimizing global memory accesses and maximizing utilization of shared memory or registers can significantly enhance performance.

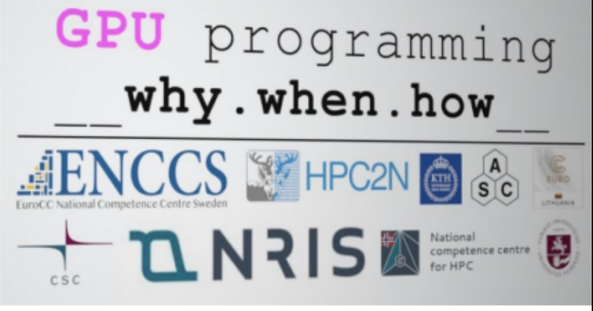
Fortran Porting Example. Code I




```
k2 = 0
do i = 1, n_sites
 do j = 1, n_neigh(i)
   k2 = k2 + 1
   counter = 0
   counter2 = 0
   do n = 1, n_max
    do np = n, n_max
     do l = 0, l_max
      if( skip_soap_component(l, np, n) )cycle

      counter = counter+1
      do m = 0, l
       k = 1 + l*(l+1)/2 + m
       counter2 = counter2 + 1
       multiplicity = multiplicity_array(counter2)
       soap_rad_der(counter, k2) = soap_rad_der(counter, k2) + multiplicity*real ( cnk_rad_der(k, n, k2)*conjg(cnk(k, np, i)) + cnk(k, n, i)*conjg
       ...
      end do
     end do
    end do
   end do
   ...
```

Fortran Porting Example. Code II




```
   ...
   soap_rad_der(1:n_soap, k2) = soap_rad_der(1:n_soap, k2) / sqrt_dot_p(i) -   soap(1:n_soap, i) / sqrt_dot_p(i)**3 * &
                              &  dot_product( soap(1:n_soap, i), soap_rad_der(1:n_soap, k2) )

   if( j == 1 )then
    k3 = k2
   else
    soap_cart_der(1, 1:n_soap, k2) = dsin(thetas(k2)) * dcos(phis(k2)) * soap_rad_der(1:n_soap, k2) - &
                                   & dcos(thetas(k2)) * dcos(phis(k2)) / rjs(k2) * soap_pol_der(1:n_soap, k2) - &
                                   & dsin(phis(k2)) / rjs(k2) * soap_azi_der(1:n_soap, k2)
    soap_cart_der(1, 1:n_soap, k3) = soap_cart_der(1, 1:n_soap, k3) - soap_cart_der(1, 1:n_soap, k2)
   end if
 end do
end do
```

False dependencies

- The loop starts with:

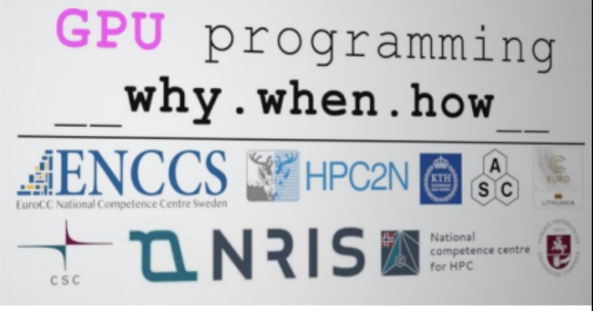
```
k2 = 0
do i = 1, n_sites
 do j = 1, n_neigh(i)
   k2 = k2 + 1
```

- Instead one can use:

```
do k2 = 1, k2_max
 i=list_of_i(k2)
```

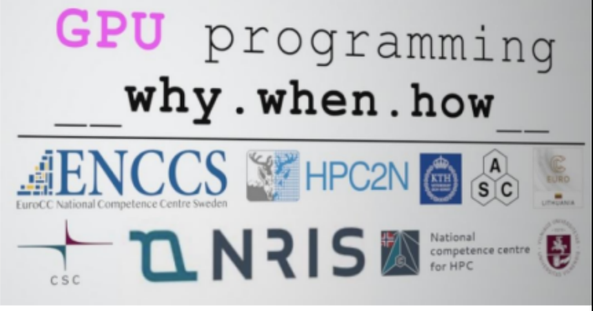
- This allows the parallization over `k2` index.

Split the Loop.



- Why ?
  - Registers are limited and the larger the kernel use more registers registers resulting in less active threads (small occupancy).
  - In order to compute `soap_rad_der(is,k2)` the cuda thread needs access to all the previous values `soap_rad_der(1:nsoap,k2)`.
  - In order to compute `soap_cart_der(1, 1:n_soap, k3)` it is required to have access to all values `(k3+1:k2+n_neigh(i))`.

Part A of the Loop




```
do k2 = 1, k2_max
 i=list_of_i(k2)
 counter = 0
 counter2 = 0
 do n = 1, n_max
  do np = n, n_max
   do l = 0, l_max
    if( skip_soap_component(l, np, n) )cycle

    counter = counter+1
    do m = 0, l
     k = 1 + l*(l+1)/2 + m
     counter2 = counter2 + 1
     multiplicity = multiplicity_array(counter2)
     soap_rad_der(counter, k2) = soap_rad_der(counter, k2) + multiplicity*real ( cnk_rad_der(k, n, k2)*conjg(cnk(k, np, i)) + cnk(k, n, i)*conjg (c
     ...
   end do
  end do
 end do
end do
...
```

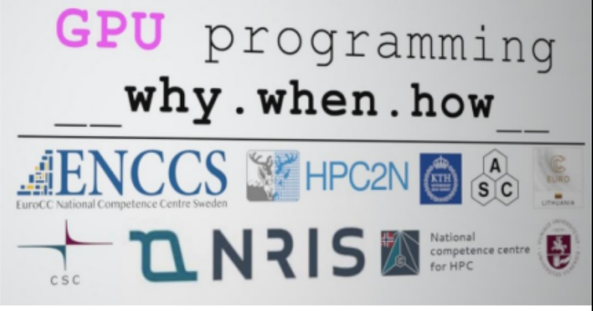
Memory Access Considerations

- Consider adjacent threads in the same block and warp.

threadIdx.x	k2	counter	soap_rad_der	cnk_rad_der
0	1	1	0	0
1	2	1	k2_max	nmax * k2_max
2	3	1	2 * k2_max	2 * nmax * k2_max

- The “most” uncoalesced way to access the memory.
- Transposing the data will result in higher performance, despite the extra operations.

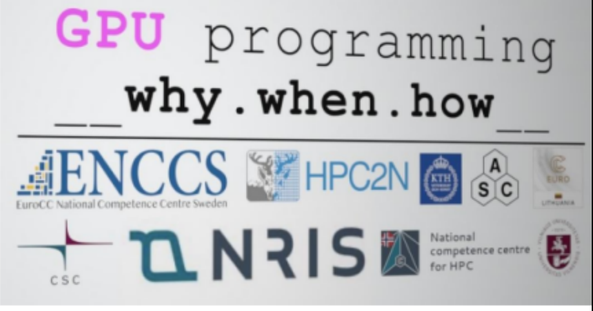
Part A with OpenMP Offloading




```
!omp target teams distribute parallel do private(i)
do k2 = 1, k2_max
 i=list_of_i(k2)
 counter = 0
 counter2 = 0
 do n = 1, n_max
  do np = n, n_max
   do l = 0, l_max
    if( skip_soap_component(l, np, n) )cycle

    counter = counter+1
    do m = 0, l
     k = 1 + l*(l+1)/2 + m
     counter2 = counter2 + 1
     multiplicity = multiplicity_array(counter2)
     tsoap_rad_der(k2,counter) = stoap_rad_der(k2,counter) + multiplicity*real ( tcnk_rad_der(k2,k,n)*conjg(tcnk(i,k,np)) + tcnk(i,k,n)*conjg (tscn
     ...
   end do
  end do
 end do
end do
...
```

Part B of the Loop



- Assuming the results were (un)transposed.

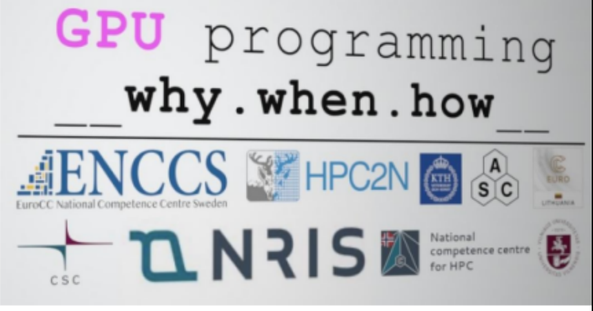
```
do k2 = 1, k2_max
 i=list_of_i(k2)

 soap_rad_der(1:n_soap, k2) = soap_rad_der(1:n_soap, k2) / sqrt_dot_p(i) -   soap(1:n_soap, i) / sqrt_dot_p(i)**3 * &
                            &  dot_product( soap(1:n_soap, i), soap_rad_der(1:n_soap, k2) )

end do
```

- We can have each thread computing one `k2` but the `dot_product( soap(1:n_soap, i), soap_rad_der(1:n_soap, k2) )` is computed `nsoap` times.
- We sacrifice memory for speed and “precompute” `dot_product( soap(1:n_soap, i), soap_rad_der(1:n_soap, k2) )`

Part B Splitted



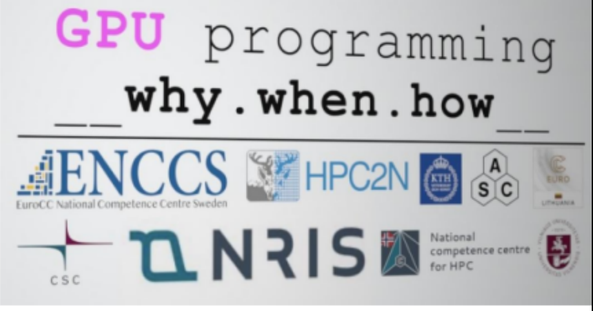

```
do k2 = 1, k2_max
 i=list_of_i(k2)
 locdot=0.d0
 do is=1,nsoap
  locdot=locdot+soap(is, i) * soap_rad_der(is, k2)
 enddo
dot_soap(k2)= locdot
end do
```

```
do k2 = 1, k2_max
 i=list_of_i(k2)

 soap_rad_der(1:n_soap, k2) = soap_rad_der(1:n_soap, k2) / sqrt_dot_p(i) -    soap(1:n_soap, i) / sqrt_dot_p(i)**3 * &
                            &  dot_soap(k2)

end do
...
```

Part B with OpenMP Offloading



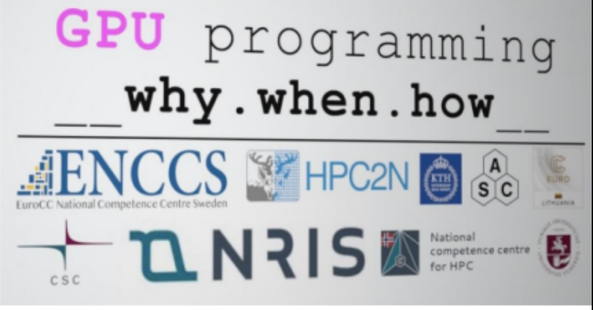

```
!omp target teams  distribute private(i)
do k2 = 1, k2_max
 i=list_of_i(k2)
 locdot=0.d0
 !omp parallel do reduction(+:locdot)
 do is=1,nsoap
  locdot=locdot+soap(is, i) * soap_rad_der(is, k2)
 enddo
dot_soap(k2)= locdot
end do
```

```
!omp target teams distribute
do k2 = 1, k2_max
 i=list_of_i(k2)

 !omp parallel do
 do is=1,nsoap
  soap_rad_der(is, k2) = soap_rad_der(is, k2) / sqrt_dot_p(i) -   soap(is, i) / sqrt_dot_p(i)**3 * dot_soap(k2)
 end do
end do
```

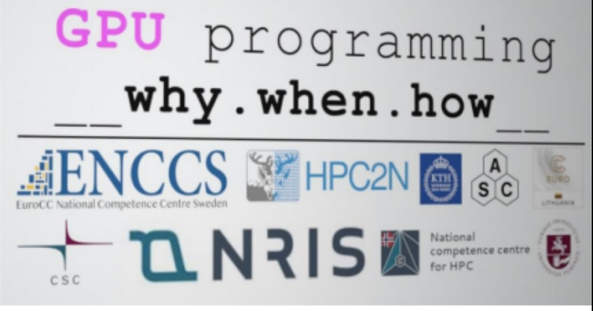
- Assuming `nsoap` ~ 100-1000. The outer loop is distributed over the blocks, while the inner loop over the threads inside of a block.

Part C of the Loop




```
do k2 = 1, k2_max
   j=list_j(k2)
   if( j == 1 )then
    k3 = k2
   else
    soap_cart_der(1, 1:n_soap, k2) = dsin(thetas(k2)) * dcos(phis(k2)) * soap_rad_der(1:n_soap, k2) - &
                                   & dcos(thetas(k2)) * dcos(phis(k2)) / rjs(k2) * soap_pol_der(1:n_soap, k2) - &
                                   & dsin(phis(k2)) / rjs(k2) * soap_azi_der(1:n_soap, k2)
    soap_cart_der(1, 1:n_soap, k3) = soap_cart_der(1, 1:n_soap, k3) - soap_cart_der(1, 1:n_soap, k2)
   end if
 end do
end do
```

Part C of the Loop Splitted

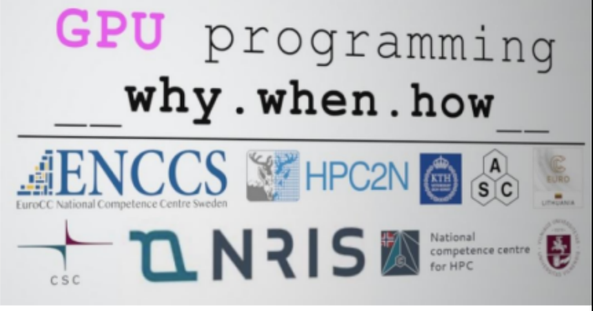



```
do k2 = 1, k2_max
 k3=list_k2k3(k2)

 if( k3 /= k2)then
   soap_cart_der(1, 1:n_soap, k2) = dsin(thetas(k2)) * dcos(phis(k2)) * soap_rad_der(1:n_soap, k2) - &
                                  & dcos(thetas(k2)) * dcos(phis(k2)) / rjs(k2) * soap_pol_der(1:n_soap, k2) - &
                                  & dsin(phis(k2)) / rjs(k2) * soap_azi_der(1:n_soap, k2)
 end if
end do
```

```
do i = 1, _sites
 k3=list_k3(i)
 do k2=k3+1,k3+n_neigh(i)
  soap_cart_der(1, 1:n_soap, k3) = soap_cart_der(1, 1:n_soap, k3) - soap_cart_der(1, 1:n_soap, k2)
 end do
end do
```

Part C of the Loop with OpenMP Offloading

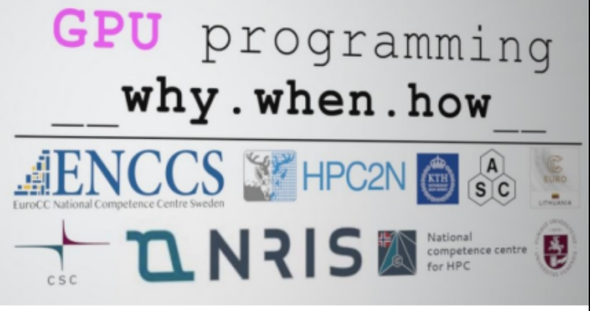



```
!omp teams distribute private(k3)
do k2 = 1, k2_max
 k3=list_k2k3(k2)

 !omp parallel do private (is)
 do is=1,n_soap
  if( k3 /= k2)then
   soap_cart_der(1, is, k2) = dsin(thetas(k2)) * dcos(phis(k2)) * soap_rad_der(is, k2) - &
                              & dcos(thetas(k2)) * dcos(phis(k2)) / rjs(k2) * soap_pol_der(is, k2) - &
                              & dsin(phis(k2)) / rjs(k2) * soap_azi_der(is, k2)
  end if
 end do
end do
```

```
!omp teams distribute private(k3)
do i = 1, _sites
 k3=list_k3(i)

 !omp parallel do private(is, k2)
 do is=1,n_soap
  do k2=k3+1,k3+n_neigh(i)
   soap_cart_der(1, is, k3) = soap_cart_der(1, is, k3) - soap_cart_der(1, is, k2)
  end do
 end do
end do
```



Summary

- Find the intensive parts for porting.
- Try to use libraries whenever possible.
- Consider refactoring of the loops.
- Check the memory access patterns
  - on CPU adjacent locations of memory need to be accessed close in time.
  - on GPU adjacent locations of memory need to be accessed by adjacent threads.
- Real life example of porting.